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# Density of States in a Resonant Tunneling Structure

by

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The change in the density of states $\Delta N(E)$ brought about by the double-barrier structure is calculated. The positions and widths of narrow resonances coincide with those obtained from transmission $T(E)$, but in many cases $\Delta N(E)$ is a better quantity for characterizing the resonances than $T(E)$.

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# Density of States in a Resonant Tunneling Structure

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## Abstract

The change in the density of states $\Delta N(E)$ brought about by the double-barrier structure is calculated. The positions and widths of narrow resonances coincide with those obtained from transmission $T(E)$, but in many cases $\Delta N(E)$ is a better quantity for characterizing the resonances than $T(E)$.

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## I. Introduction

Resonant tunneling structures (RTS) are exciting systems because of their potential applications, but also because of the basic physics they involve. In particular, the times related to the tunneling process have been the subject of theoretical disputes.[1] The dwell times and transmission times can be extracted from optical or transport experiments. These times can be found from the study of wave-packet propagation from the time-dependent Schrödinger equation, but they can also be related to some static characteristics of the RTS (see, e.g., Ref. 2 and references therein). Most commonly the lifetime of the resonance state is determined from the halfwidth of the energy derivative of the phase shift or, equivalently, from the transmission coefficient T(E). Here we would like to calculate another important static quantity characterizing the RTS, namely the change in the density of states $\Delta N(E)$ that it introduces. As shown for scattering resonances in three dimensions, the position and width of the narrow peaks in cross-sections are the same as in the density of states (see,e.g., the discussion for the short-range potentials in Ref. 3). Therefore, in our one-dimensional case we expect the resonances in $\Delta N(E)$ to coincide with those in T(E). Of course, in the nonresonant regions the two quantities can be very different. There are cases, however, when the transmission cannot be used to describe resonant states. Two such examples are shown in Fig. 1 -- there is no transmission at the resonance energy. The density of states $\Delta N(E)$ could still be used to characterize such systems. Another possibility would be the analysis of the phase shifts in reflection or the study of wavefunctions in the complex energy plane,[4,5] but we believe that $\Delta N(E)$ is the most basic physical quantity characterizing the continuous spectrum.

In the present paper we calculate $\Delta N(E)$ for an asymmetric double-barrier structure without bias, but the method can be generalized to other cases. The local density of states in the double-barrier structure has recently been obtained[6,7] and analyzed for various limits. It can be defined as

$$N(E,x) = \sum_n \delta(E-E_n) \; |\psi_n(x)|^2 \tag{1}$$

where $E_n$ are the eigenvalues of the system and $\psi_n$ are the corresponding eigenstates. Equation (1) has been integrated in Ref. 6 over the volume of the "well" in the RTS. Such quantity depends on the region of integration. It is modified by the RTS due to: (i) modification of the wavefunctions (ii) change of the position of energy levels $E_n$. In Ref. 6 the second modification has been neglected, i.e., their $\Delta N(E,x)$ would be identically zero if integrated over the total volume. Here we want to consider the global density of states

$$N(E) = \sum_n \delta(E-E_n) \quad , \tag{2}$$

which is modified by the RTS only through the change of spacing of the energy levels and does not involve any specific region in space.

## II. Determination of $\Delta N(E)$

In order to deal with finite densities of states, we must place our RTS in a large box extending, say, from 0 to L. In an empty box, the condition for the energy levels ($E = \frac{\hbar^2 k^2}{2m}$) is

$$D_o(k) = \sin kL = 0 \quad , \tag{3}$$

which yields $k_n = n\frac{\pi}{L}$, i.e., equally-spaced points in k-space. The density of states is the inverse of the spacing between the points,

$$N_o(k) = \frac{L}{\pi} \quad , \tag{4}$$

and is proportional to the size of the box. In the presence of the RTS, the condition for the energy levels is modified to

$$D(k) = 0 \quad , \tag{5}$$

where we use the same definition of $k(E = \frac{\hbar^2 k^2}{2m})$ as before. The condition $D(k) = 0$ above is obtained by demanding that the wave function $\psi(x)$ vanishes at the right edge $(x = L)$ of the box. We start with the solution $\psi(x) = \sin kx$ near the left edge $(x = 0)$ of the box and require the usual continuity of this wave function and its first derivative across the first interface. This matching condition determines the two unknown coefficients of the solutions to the Schrödinger equation to the right of the first interface. We repeat the procedure until the most general solution on the right-hand side region of the last interface is obtained. Finally, imposing the boundary condition that at $x = L$ the wave function must vanish gives the required condition. The function $D(k)$ is given in the Appendix for the case of an asymmetric double-barrier structure, but it can be determined for any other potential profile. Now the spacing between the points in k-space is altered, althouth only by an extremely small amount, because we expect $\Delta N(E)$ to be finite while $N_o(E)$ will

increase linearly with the box size. Thus, we expect, for instance, to find in some energy region 10001 states in the presence of the RTS and 10000 without it. This means that the spacing $\Delta k_n$ will be almost identical to $\frac{\pi}{L}$ for large L,

$$\Delta k_n = \frac{\pi}{L} + x_n \quad , \tag{6}$$

where $x_n << \frac{\pi}{L}$. The change in the density of states becomes

$$\Delta N(k_n) = N(k_n) - N_o(k_n) = \frac{1}{\Delta k_n} - \frac{L}{\pi} \simeq -(\frac{L}{\pi})^2 x_n \quad . \tag{7}$$

We expect $\Delta N$ to tend to a constant with increasing box size, so that $x_n$ should be of the order of $(\frac{\pi}{L})^2$.

Now we have to determine $x_n$ from Eq. (5). Suppose the box is large enough and we find the first eigenstate at $k = k_1$. The next root of D(k) should occur at $k_2 = k_1 + \frac{\pi}{L} + x_1$. Due to the smallness of $x_1$, we get

$$x_1 \simeq - \frac{D(k_1+\frac{\pi}{L})}{D'(k_1+\frac{\pi}{L})} \quad . \tag{8}$$

The next root will be at $k_3 = k_2 + \frac{\pi}{L} + x_2$, and again

$$x_2 \simeq - \frac{D(k_2+\frac{\pi}{L})}{D'(k_2+\frac{\pi}{L})} \quad . \tag{9}$$

Here we notice that although $x_1, x_2, \ldots$ are small, they may add up to something large, so that the shift cf $k_n$ with respect to $k_n^o = n\frac{\pi}{L}$ may be substantial. The spacing of the levels $\Delta k_n$ will be almost identical to $\Delta k_n^o = \frac{\pi}{L}$.

The above prescription for finding $\Delta N(k)$, and therefore $\Delta N(E)$,

$$\Delta N(E) = \Delta N(k) \frac{m}{\hbar^2 k} \quad , \tag{10}$$

is very simple. The only problem with it is that it does not work. If we look at the positions of the roots of D(k), we find very irregular spacing, different from $\frac{\pi}{L}$ even for a very large box and strongly dependent on the positions of the RTS in the box. In other words, the shifts of the levels due to the RTS depend on the phase with which the wavefunction reaches the structure. This can be understood if we look at the problem differently. Suppose we have a single thin barrier in the middle of the box. With respect to the center of the box, all states are either symmetric or antisymmetric. It is obvious that the barrier affects each type differently. Therefore, we can expect to get two "subdensities" of states -- one corresponding to symmetric and the other to antisymmetric states. For each of these subdensities, the above described method for finding $\Delta N(E)$ can be applied, but not to the total density of states. For other positions of the structure in the box, the number of subdensities will be higher: if the RTS is placed at $\frac{L}{3}$, we get three subdensities, and if it is at 0.4 L, we get five subdensities. The number of subdensities equals the number of possible phases with which the wavefunction can reach the RTS. The superposition of several equally-spaced subsets of points in k-space results in something that looks messy. But

applying our method to each subdensity and then adding them all up gives us $\Delta N(E)$ independent of the position of RTS in the box, as could be expected.

The procedure is thus as follows: we place the RTS at a given point in the box, say, at $\frac{L}{3}$. This means that we have three subdensities -- we start from some initial energy and find three subsequent roots of $D(k)$. Each of these roots defines a subset of states with the spacings equal to $\frac{\pi}{(3L)} + x_n$, where $x_n$ is very small. We determine

$$x_n \simeq - \frac{D(k_n + \frac{\pi}{3L})}{D'(k_n + \frac{\pi}{3L})} \tag{11}$$

for each subdensity and then $\Delta N(k_n)$ from Eq. (7) (with L replaced by 3L). Adding up the three subdensities, we get the final result. The size of the RTS is usually of the order of 100 Å, while the box size must be $10^4$ - $10^7$ Å depending on how fine the structures are (narrow resonances) in $\Delta N(E)$ which we want to consider.

## III. Results and discussion

Let us start from the single-barrier case with $D(k)$ given by Eq. (A2) in the Appendix. We assume $m = 0.067\ m_o$ throughout the structure. In Figure 2 we show the transmission $T(E)$ and the change in density of states $\Delta N(E)$ for single barriers 100 meV high and 50 Å wide (Fig. 1a) or 100 Å wide (Fig. 1b). In the first case both $T(E)$ and $\Delta N(E)$ do not show any sharp structures; transmission increases almost monotonically from zero to one as expected. In the second case transmission oscillates before it reaches unity while $\Delta N(E)$ exhibits a distinct (though broad) resonance. For low energies $\Delta N(E)$ is

negative as if some levels were pushed up from below the barrier and "piled up" above its top.

Next we look at a double-barrier structrue with D(k) given by Eq. (A1) in the Appendix. First we consider a symmetric RTS with barriers 50 Å wide and 200 meV high, and the well being 100 Å wide. There are two quasi-bound states in the well and several resonances above the barriers. In Figure 3 we show three resonances having the same position and width in T(E) and in $\Delta N(E)$. We note the different vertical scales for different resonance in $\Delta N(E)$. The transmission always varies between zero and one (it reaches one for a symmetric structure) while the peaks in $\Delta N(E)$ correspond to single bound states, i.e., $\int \Delta N(E)dE \approx 1$ for each peak. Therefore broader peaks in $\Delta N(E)$ are much lower than the narrow ones. Away from the resonances $\Delta N(E)$ often becomes negative -- the states are depleted from some regions and piled up in other regions. Transmission, of course, is always positive.

Figure 4 shows T(E) and $\Delta N(E)$ for the same structure as in Fig. 3 but for higher energies. Again we can see wiggles in transmission and distinct resonances in $\Delta N(E)$. In Fig. 5 we give another example of the same behavior; this time we consider an asymmetric structure with 50 Å barriers and 50 Å well but the first barrier is 100 meV high while the second is 200 meV high. Around 200 meV there is a peak in $\Delta N(E)$ and only the inflection point in T(E).

Concluding, we have found a simple method for calculating the global density of states (and its change $\Delta N(E)$) in a resonant tunnelling structure. We believe that $\Delta N(E)$ is a much better characteristics of resonant states than transmission and it can be applied to more general cases (see Fig. 1). In such cases our method should be modified - the unperturbed density of states in k-space $N_o(k)$ will not be uniform. For the structures in Fig. 1 the

unperturbed structure would include a potential step. The spacing of the levels would then be modified by the presence of RTS.

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Appendix: Energy levels in a box containing the RTS

Consider the double-barrier structure placed in a large box extending from 0 to L. The first barrier extends from $x_1$ to $x_1 + a_1$ with a height of $V_1$ and the second from $x_2 = x_1 + a_1 + d$ to $x_2 + a_2$ with a height of $V_2$. We assume a constant effective mass across the structure. The boundary conditions (continuity of the wavefunction and its first derivative) at four interfaces (and at the edges of the box) yield the following condition for the bound states:

$$
\begin{aligned}
D(k) = {} & \cos\kappa_2 a_2\Big[\sinh(\kappa_1 a_1)\Big(\frac{\kappa_1}{k}\sin(kx_1)\sin(k(y+d)) \\
& + \frac{k}{\kappa_1}\cos(kx_1)\cos(k(y+d))\Big) + \cosh(\kappa_1 a_1)\sin(k(x_1+y+d))\Big] \\
& + \sinh(\kappa_2 a_2)\Big\{\sinh(\kappa_1 a_1)\Big[\sin(kd)\Big(\frac{\kappa_1\kappa_2}{k^2}\sin(ky)\sin(kx_1) \\
& - \frac{k^2}{\kappa_1\kappa_2}\cos(ky)\cos(kx_1)\Big) + \cos(kd)\Big(\frac{\kappa_1}{\kappa_2}\cos(ky)\sin(kx_1) \\
& + \frac{\kappa_2}{\kappa_1}\sin(ky)\cos(kx_1)\Big)\Big] + \cosh(\kappa_1 a_1)\Big[\frac{\kappa_2}{k}\sin(ky)\sin(k(x_1+d)) \\
& + \frac{k}{\kappa_2}\cos(ky)\cos(k(x_1+d))\Big]\Big\} = 0 \quad , \qquad \text{(A1)}
\end{aligned}
$$

where $\frac{\hbar^2 k^2}{2m} = E$, $\frac{\hbar^2\kappa_1^2}{2m} = V_1 - E$, $\frac{\hbar^2\kappa_2^2}{2m} = V_2 - E$, $y = L - a_2 - x_2$. For a single barrier extending from $x_1$ to $x_1 + b$, we get a simpler expression,

$$
D(k) = \cosh(\kappa b)\sin(k(L-b)) + \sinh(\kappa b)\Big(\frac{k}{\kappa}\cos(kx_1)\cos(k(x_1+b-L))
$$

$$-\frac{\kappa}{k}\sin(kx_1)\sin(k(x_1+b-L))\Big\} = 0 \quad . \qquad \text{(A2)}$$

The above formulas are valid for $E < V_1$ and $E < V_2$. If the energy is above any of the barriers, say $E > V_1$ we make the replacement

$$\kappa_1 \rightarrow ik_1 \quad , \quad \sinh\kappa_1 a_1 \rightarrow i\sin k_1 a_1 \quad , \quad \cosh\kappa_1 a_1 \rightarrow \cos k_1 a_1 \quad . \qquad \text{(A3)}$$

The expression for D(k) is always real, i.e., the imaginary constants cancel.

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## Figure Captions

1. Two examples of structures involving resonant states that could be studied in terms of $\Delta N(E)$ but not in terms of transmission $T(E)$: (a) strongly biased, wide double-barrier structure and (b) single well with finite width barrier on one side. The resonance is indicated by a shaded area.
2. Transmission $T(E)$ and density of states $\Delta N(E)$ for a single barrier 100 meV high and 50 Å wide (a) or 100 Å wide (b).
3. Transmission $T(E)$ and density of states $\Delta N(E)$ in various energy regions for a symmetric double-barrier structure. The barriers are 50 Å wide and 200 meV high, and the well is 100 Å wide.
4. Same as in Fig. 3 but for higher energies. Note the resonances in $\Delta N(E)$ and wiggles in $T(E)$.
5. Transmission $T(E)$ and density of states $\Delta N(E)$ in the energy region above the lower barrier for an asymmetric double-barrier structure. The barriers and the well are each 50 Å wide. The first barrier is 100 meV high, and the second is 200 meV high. Note the peak is $\Delta N(E)$ at about 200 meV and the corresponding "blob" in $T(E)$.

Fig

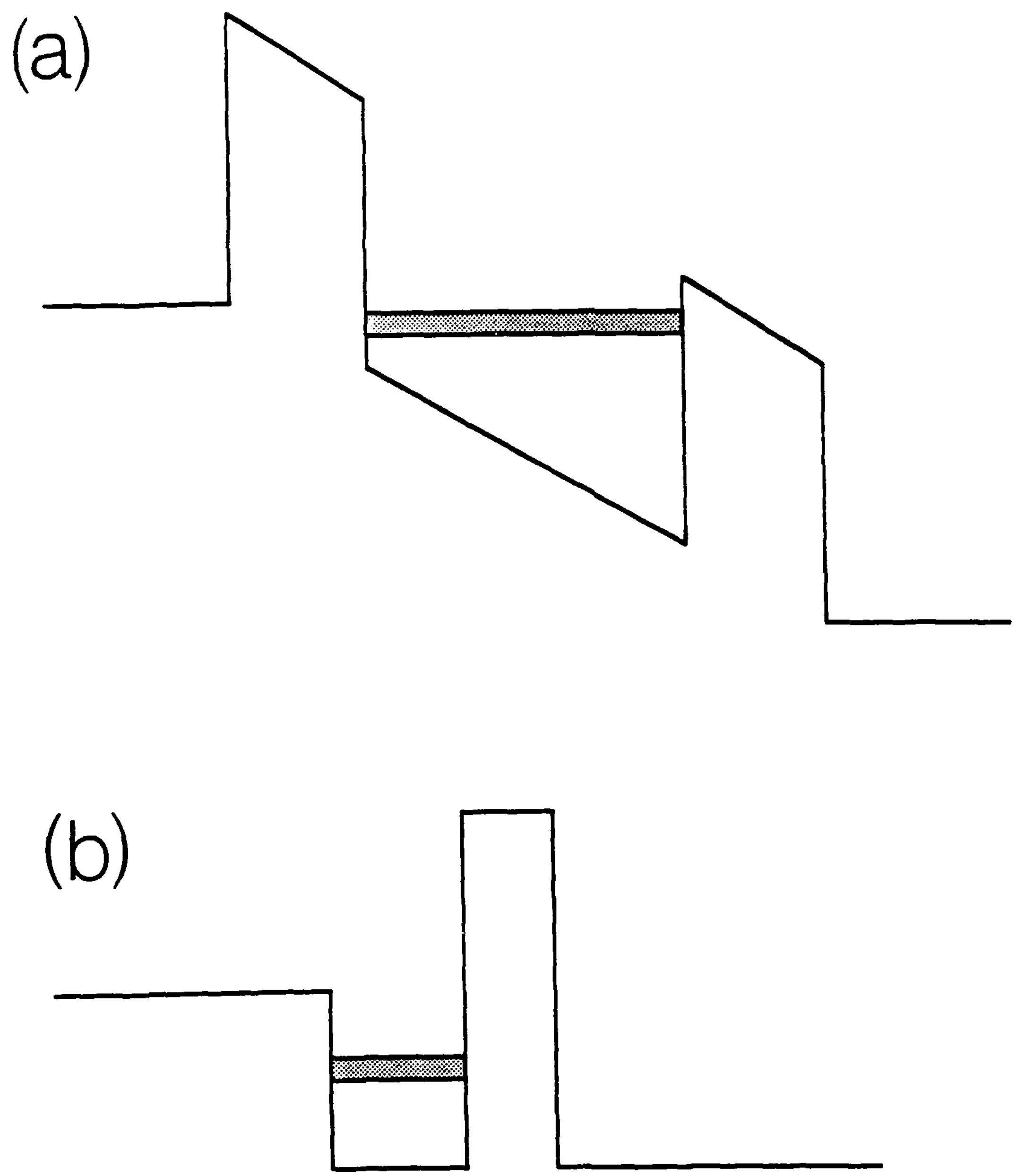


Fig. 2 (a)

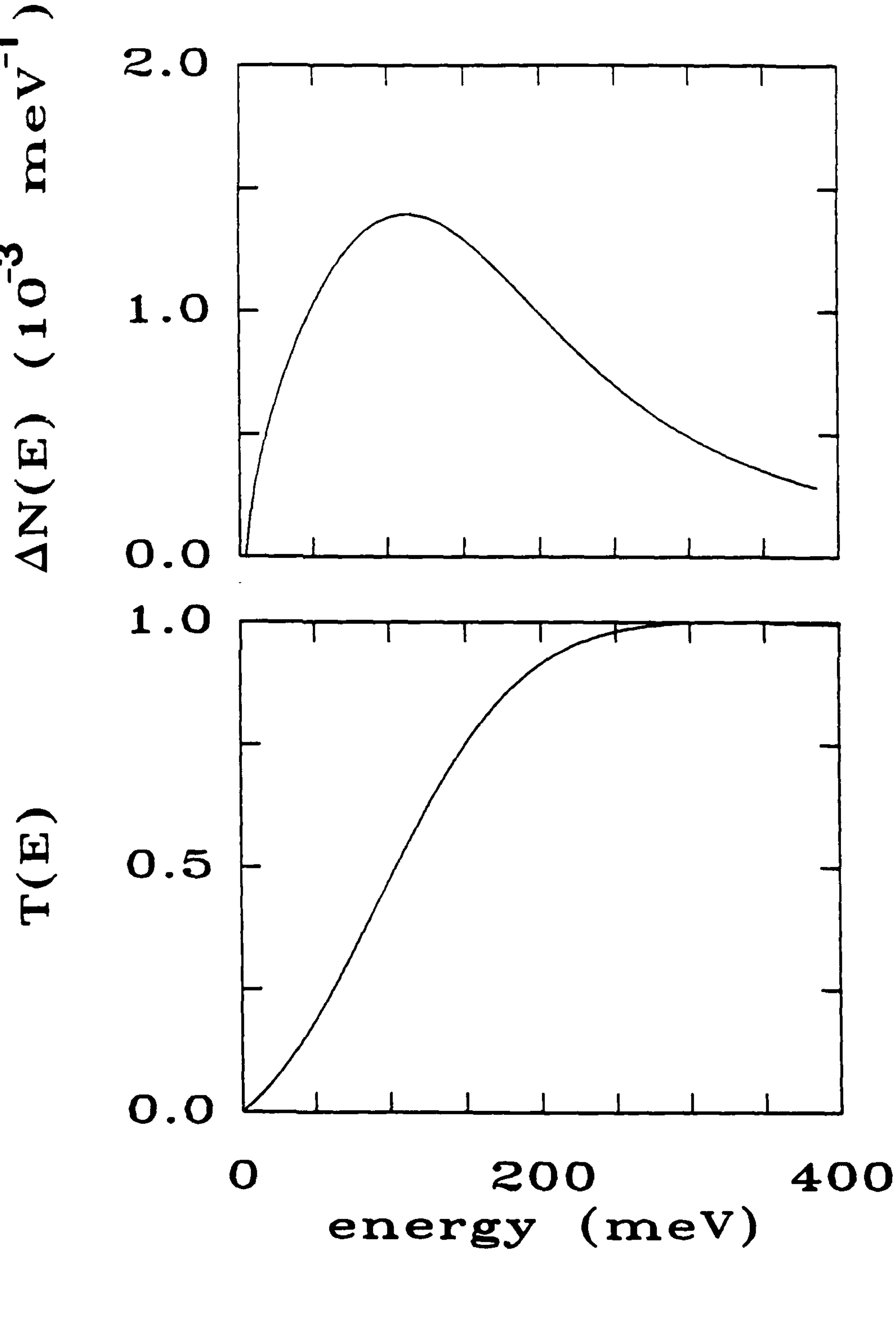


Fig. 2 (b)

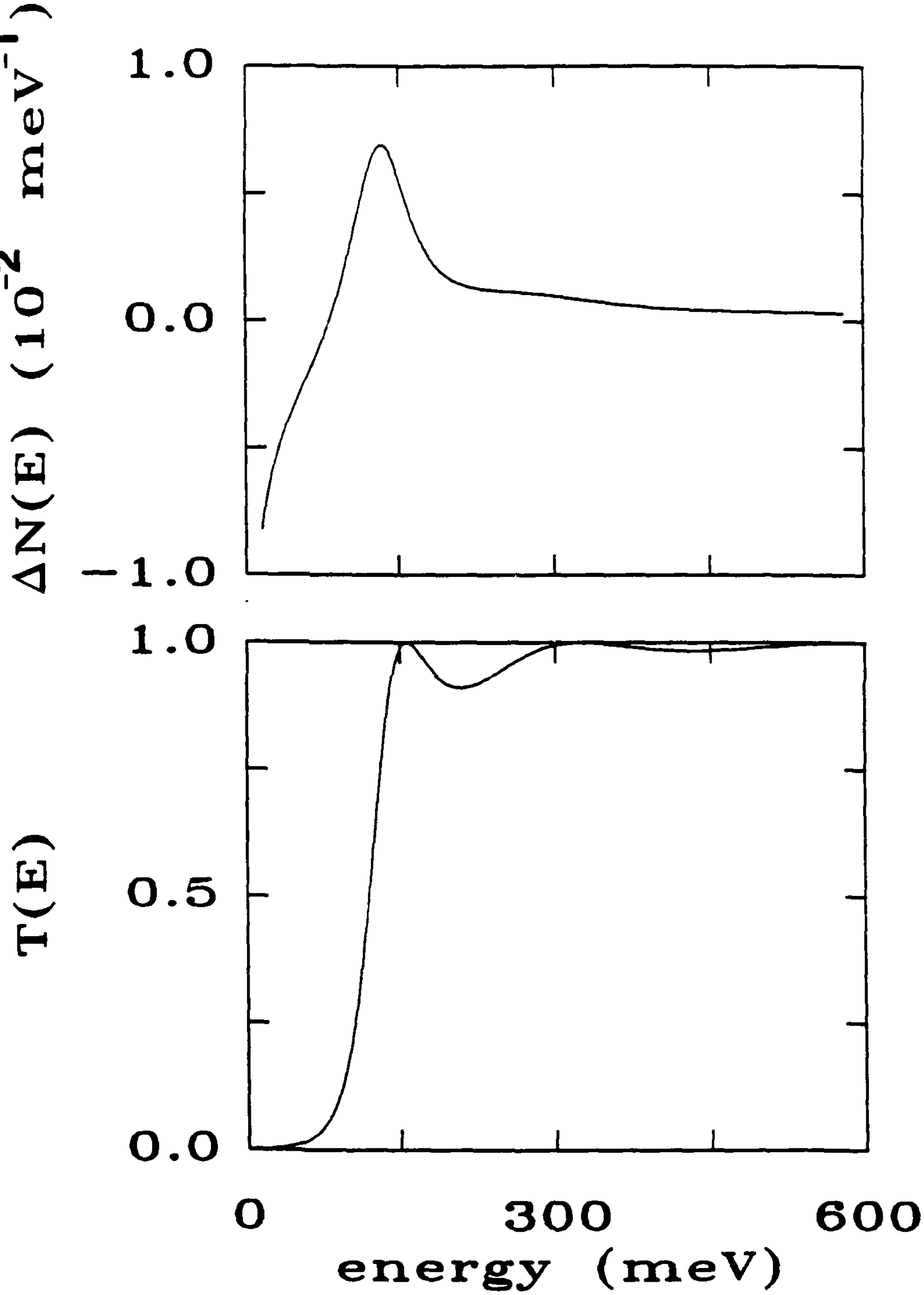


Fig 3

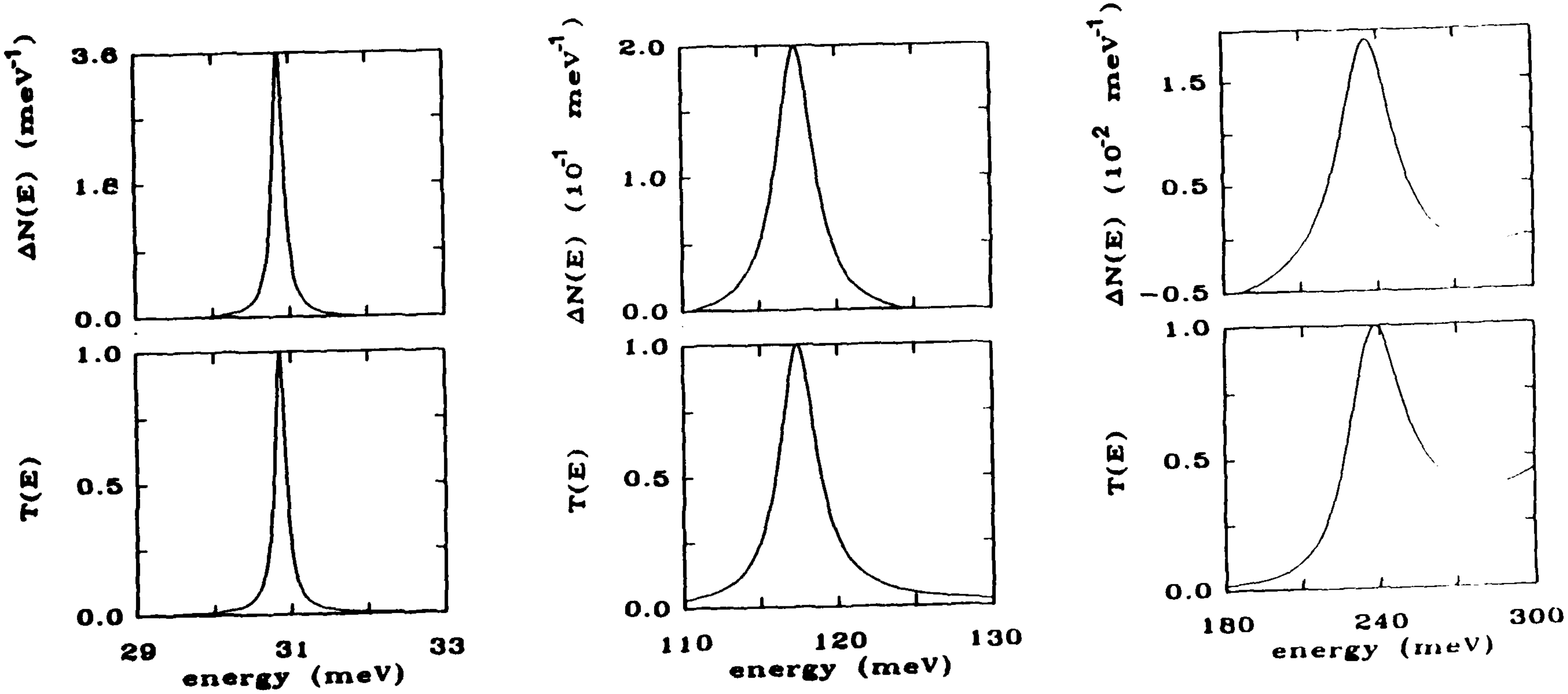

ΔN(E) (meV⁻¹)
3.6
1.8
0.0
T(E)
1.0
0.5
0.0
29
31
33
energy (meV)
ΔN(E) (10⁻¹ meV⁻¹)
2.0
1.0
0.0
T(E)
1.0
0.5
0.0
110
120
130
energy (meV)
ΔN(E) (10⁻² meV⁻¹)
1.5
0.5
−0.5
T(E)
1.0
0.5
0.0
180
240
300
energy (meV)

Fig. 4

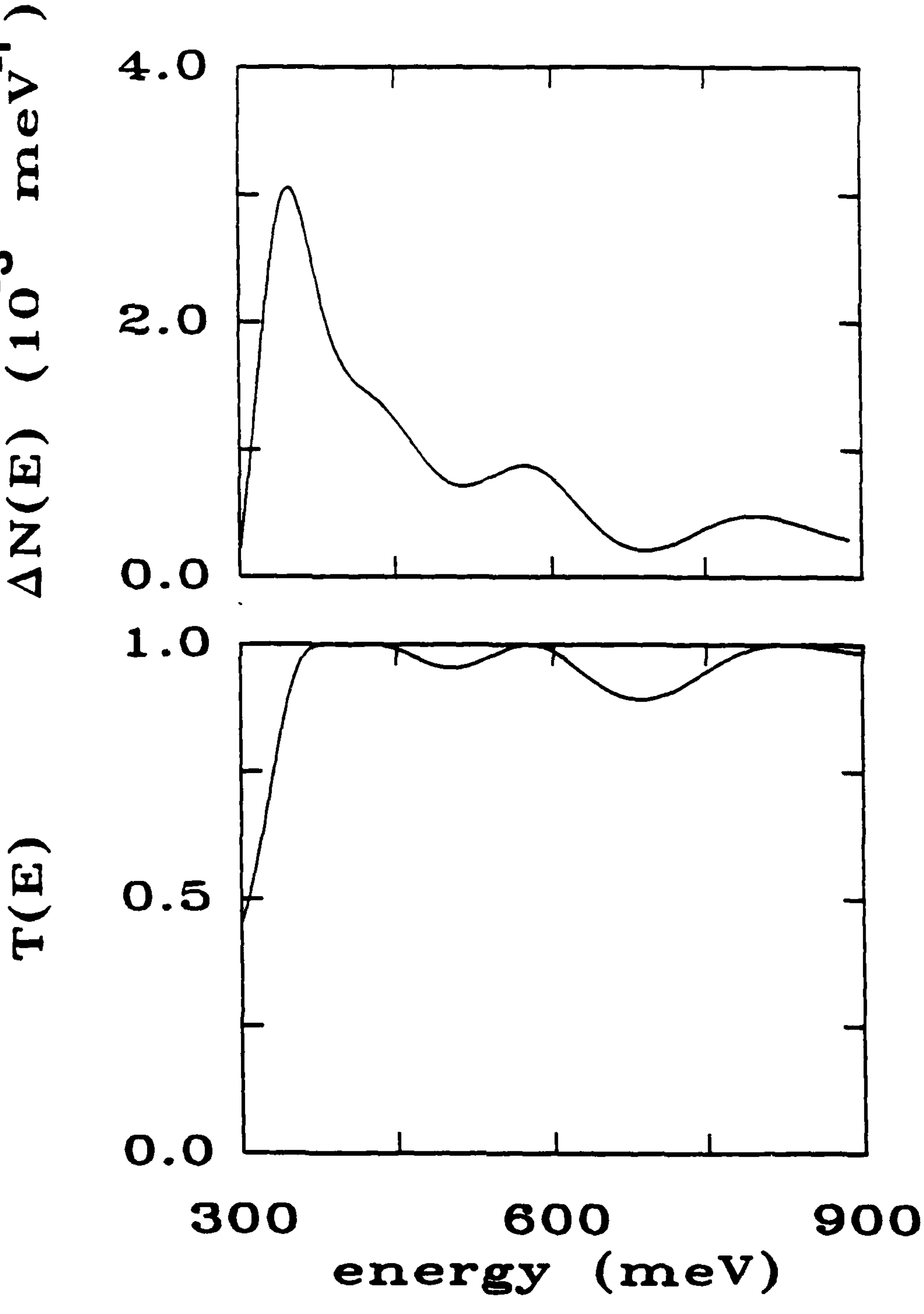
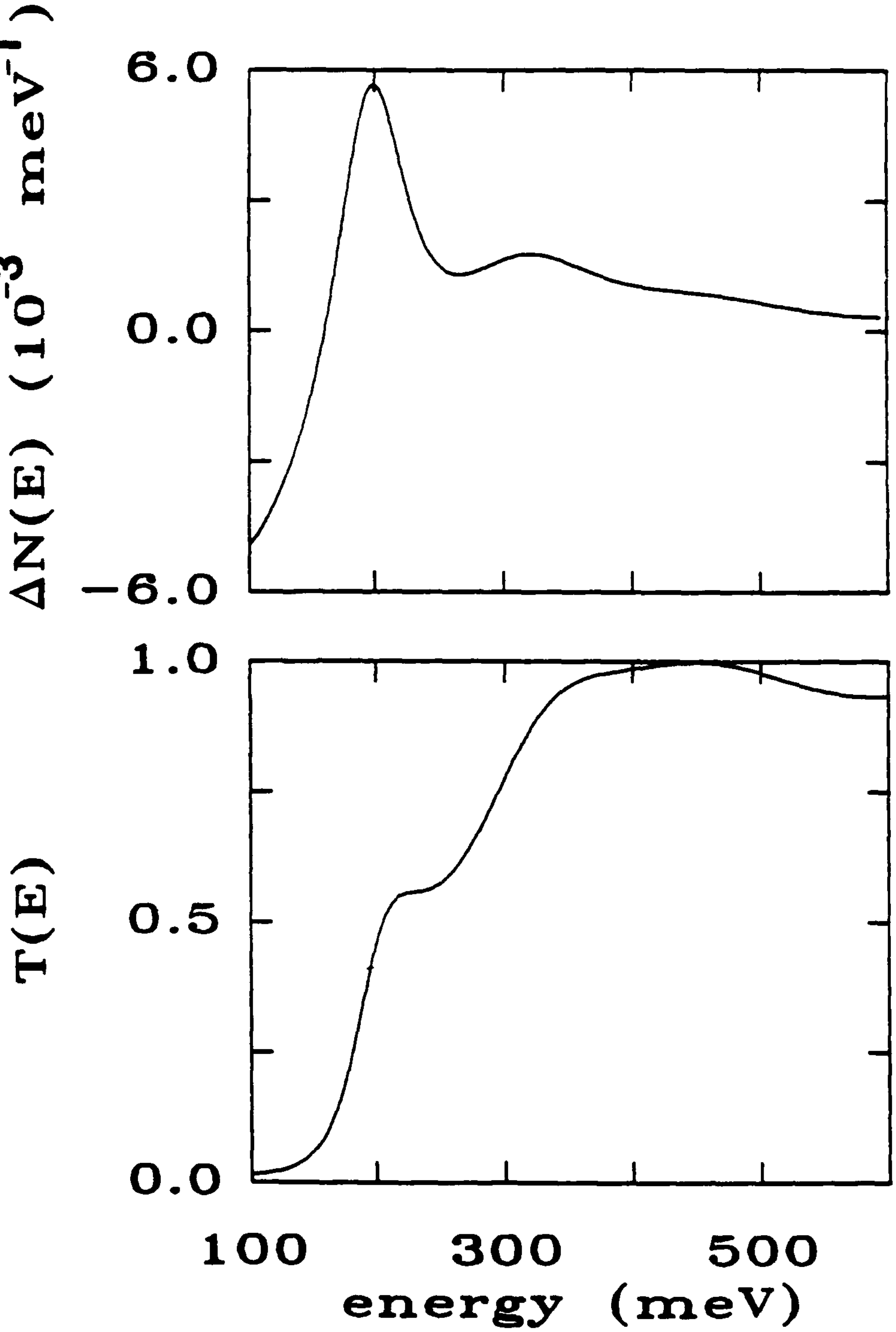


Fig. 5



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